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DATA SCREENING AND CALCULATION PROCEDURES FOR THE NORTH AMERICAN PRECIPITATION CHEMISTRY DATA TO BE USED IN THE INTERNATIONAL SULFUR DEPOSITION MODEL EVALUATION

by

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16. ABSTRACT

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Since the methods for quality control and quality assurance of the precipitation chemistry data and procedure for computing wet deposition amounts are not always in agreement between the networks, it was necessary to adopt unified procedures for screening/correcting the data and computing deposition amounts. A scheme was also developed for estimating the uncertainties in the wet deposition amounts.

The procedures for computing wet deposition amounts and estimating the associated uncertainties are described and results from five networks in eastern North America are given.

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Since the methods for quality control and quality assurance of the precipitation chemistry data and procedure for computing wet deposition amounts are not always in agreement between the networks, it was necessary to adopt unified procedures for screening/correcting the data and computing deposition amounts. A scheme was also developed for estimating the uncertainties in the wet deposition amounts.

The procedures for computing wet deposition amounts and estimating the associated uncertainties are described and results from five networks in eastern North America are given.

1. Introduction

Long Range Transport of Air Pollutant (LRTAP) models have been developed within the last decade to estimate sulfur dioxide and sulfate concentrations, wet, dry and total sulfur deposition across Europe and North America. The results from these models have been used to estimate source-receptor relationships on a regional and international scale and as input for evaluation of control strategies and emission reduction scenarious.

Since the results from these models do not always agree it is important that the models are evaluated against network data to assess model credibility. During the US/Canadian Memorandum of Intent (MOI) on Transboundary Air Pollution[1] an attempt was made to evaluate eight Lagrangian Sulfur Deposition models against network data for 1978. Since these data were neither of sufficient quantity nor quality to allow discrimination between the models, it was recommended that the model evaluation would be extended to a period when precipitation chemistry data were more abundant.

The International Sulfur Deposition Model Evaluation (ISDME) is a direct response to the MOI recommendations. The scope of the study is described in detail by Clark et al.[2]. Seasonal and annual ambient air concentrations of sulfur dioxide and sulfate as well as wet sulfur deposition amounts over eastern North America for 1980 predicted by twelve LRTAP models, developed in Europe and North America, will be statistically intercompared. The model results will also be statistically compared with deposition amounts derived from observations from the Air and Precipitation Monitoring Network (APN) and Canadian Network for Sampling Precipitation (CANSAP) in Canada and from the Electric Power Research Institute's - Sulfate Regional Experiment (EPRI - SURE), Multistate Atmospheric Power Production Pollution Study (MAP3S) and National Atmospheric Deposition Program (NADP) in the United States. The APN, EPRI-SURE and MAP3S networks collect precipitation on an daily basis, the NADP network on a weekly and the CANSAP network on a monthly basis.

For a meaningful intercomparison between regional models and network data, it is important that the wet deposition amounts estimated from the different networks are comparable, that the uncertainties in the observed amounts are known and that only regionally representative sites are considered.

Since the methods for quality control and quality assurance of the precipitation chemistry data and procedure for computing wet deposition amounts are not always in agreement between the above mentioned networks, it was necessary to adopt a unified procedure for screening/correcting the data and computing deposition amounts. Also, since the wet deposition amounts estimated at the different monitoring sites may not be of the same quality, a scheme was developed to classify the data into different levels of uncertainty. The level of uncertainty is based on the deviation of the location of a monitoring site from ideal siting criteria, on the amount of data capture, sampling efficiency and on the contamination from sea spray.

The methods of data screening/correcting, calculation of wet deposition amounts and assessment of uncertainties are being refined and expanded to other networks by the "Unified Data Base Committee" established under the Canadian Federal-Povincial Research and Monitoring Co-ordinating Committee's Atmospheric Science Sub-Group (RMCC/ASSG)[3]. The committee intends to compute seasonal and annual wet deposition amounts for the period 1980-82.

This paper summarizes the approach taken in ISDME to compute wet depositions from the above networks, and for assessing uncertainties. It also gives screening results for wet deposition of sulfate for 1980.

2. Calculation of Concentration and Deposition

2.1 Concentration in precipitation and wet deposition amount are computed on an annual and seasonal basis, where winter is defined as January - March and other seasons accordingly.

2.2 The seasonal/annual precipitation weighted concentration ($\bar{C}$) is computed as

$$\bar{C} = \frac{\sum_{1}^{n} C_i P_i}{\sum_{1}^{n} P_i}$$

where

C_i = concentration measured during collection period i (event, week, month)

P_i = precipitation recorded during collection period i (see 2.4).

n = number of simultaneous measurements of precipitation and concentration during the season/year.

2.3 The seasonal/annual wet deposition amount (D) is computed as the product of the precipitation weighted mean concentration ($\bar{C}$) and the total precipitation for the season/year (P_T)

$$D = \bar{C} \cdot P_T$$

where

$$P_T = \sum_{1}^{N} P_i$$

P_i = precipitation recorded during collection period i

N = number of collection periods during the season/year

2.4 Precipitation (P_i) recorded during collection period(i) is generally the amount recorded by a co-located standard rain or snow gauge (Ps). If the co-located rain or snow gauge amount is missing, then the value recorded by a representative climatological rain or snow gauge (Psc) is used for the Canadian networks. For the US networks the precipitation chemistry collector amounts are used when the rain gauge amounts are not available.

2.5 The validity of a sample is judged from the data flags and field/laboratory comments in the actual data bases. Thus samples affected by sampler malfunctions, contaminated samples, bulk samples, long period samples etc. have been ignored. Valid samples, below the detection limit, have been assigned a value of half the detection limit.

3. Data Screening Criteria

Ideally one would like to quantify the uncertainty in the deposition amounts. Since, at this stage no agreed upon method has been published, the data have been classified into three levels of uncertainties based on location of the sampler, collection efficiency, number of recorded sampling periods and degree of seasalt contaminations. The criteria are given in Tables 1 to 3.

land-use pattern in the region surrounding the sites, the strength and location of the sources ("upwind"/"downwind" of sampler) and performance of the networks were considered (Vet, pers. comm.) fourteen CANSAP and six APN sites were deemed suitable for evaluation purposes. These sites were reclassified as representative and graded "good" and "fair, where the "good" sites were those meeting the criteria in Table 4. Eight of the unrepresentative sites were located in urban areas or in the vicinity of construction sites. These were, therefore, totally unsuitable for evaluation purposes and the potentially unrepresentative sites were classified into "poor" and "unsuitable".

Due to lack of available information on the siting of the US networks criteria 3-7 were not used for the US sites. Thus only proximity to and strength of emissions sources were considered. Emission data were obtained from Version 2 of the 1980 National Acid Precipitation Assessment Program Emission Inventory. Four of the nine EPRI-SURE, one of the eight MAP3S and twenty-eight of the fifty-five NADP sites were classified as representative. This rating might be modified, when comments from network personnel become available. The distribution and classification of the US and Canadian sites are given in Figure 1. The Figure shows a grading of the Canadian sites in the representative and unrepresentative categories, i.e.."good" and "fair" and "poor" and "unsuitable", respectively. The "unsuitable" sites are labelled "bad" in the Figure. The US sites in the representative category are shown as "good" and in the unrepresentative category as "poor".

4.2 Disregarding the siting criterion (Tables 1-3, criterion 1) and considering only sea salt correction, collection efficiency and number of samples, i.e. the level of observation, it was found that of the four reporting APN sites, all but one site met the seasonal and annual level 1 criteria. Twelve of the twenty-one CANSAP (i.e. excluding "unsuitable") sites met the annual level 1 criteria, eleven met the seasonal level 1 criteria in winter and spring, fourteen in summer and five in fall. None met the annual level 2 criteria, while in winter, spring, summer and fall, five, three, two and five sites, respectively, fell into level 2. When in addition siting was taken into account (i.e. all criteria in Tables 1-3) only eight sites met the annual level 1 criteria, seven met the seasonal criteria in winter, six in spring, nine in summer and five in fall. The level 2 distribution was zero, three, three, two and three, respectively. The most frequent reasons for failing level 1 and 2 were siting and poor collection efficiency.

In the MAP3S and EPRI-SURE networks all but three sites met the seasonal and annual level 1 criteria for observations. These three sites met level 2 criteria. When taking siting into account, only one of the MAP3S and four of the EPRI-SURE qualified as level 1.

Sampling at several NADP sites was initiated in 1980. Thus only fourteen sites met annual level 1 criteria for observations (Tables 1-3, excluding criterion 1). Of the reporting sites between fifty and seventy percent met level 1 and about ten percent met level 2 seasonal criteria. These percentages were reduced to about thirty and five, respectively when siting was considered. The failure to meet the criteria were primarily due to siting and poor data capture. Under-catch is only a minor problem in the US networks. However, several of the collectors in the three networks showed over-catch. Extreme values of annual and seasonal over-catch of more than one hundred and seventy and two hundred and fifty percent, respectively were recorded in the MAP3S and NADP networks.

In Figures 1-5, the rating of the sites and the level of observations at the sites are given for the year 1980 as well as for the individual seasons. The rating is indicated by a symbol, while the level of observation, when

Data falling into level 3 are judged to have the highest uncertainty.

3.1 The sites are classified into two categories, viz. representative and potentially unrepresentative for estimating regional deposition. The rating of a site is based on its location relative to objects that may interfere with collection efficiency and sources of pollutants. The criteria for a regionally representative site are given in Table 4. The different networks mentioned in the introduction use, with some deviation, similar criteria.

3.2 Precipitation concentrations measured at sites within 100 km of the coast are adjusted for sulfate contribution from sea spray. The uncontaminated sulfate concentration is estimated using the relationship[4]:

$$(SO_4^{2-})_{corrected} = (SO_4^{2-})_{observed} - 0.25\ (Na^+)_{observed}$$

where concentrations are in mg/l. Depending on the amount of correction the sample falls into level 1-3.

The percent corrections in Tables 1-3 refer to the overall period (season/annual). Thus corrections for individual samples may exceed the criteria for the period.

3.3 The overall collection efficiency (C.E.) is the ratio of the precipitation measured by the collector (Pc) and the co-located rain gauge (Ps) during the season or year.

$$C.E. = \frac{\sum_{1}^{n} Pc}{\sum_{1}^{N} Ps}$$

where n, N are defined in 2.2 and 2.3. If the co-located rain gauge value is missing the amount from a representative climate station is used. The percent collection efficiency in Tables 2-3 refers to the season. Thus collection efficiency for individual samples may fall below the seasonal criteria.

3.4 The overall collection efficiency requirements for winter and thus for the year in Canada are lower than in the United States. During the winter a large amount of the precipitation in Canada is in the form of snow resulting in poor collection. It is believed that the poor collection is due to undercatch rather than malfunction of the collector, resulting in a reasonably representative sample. This assumption is currently under investigation.

4. Results

4.1 The sites from the APN and CANSAP networks were classified according to the criteria outlined in Table 4. The site descriptions were used to determine proximity to storage facilities, major transportation sources, agricultural activities, trees etc. as well as to identify ground cover (i.e. criteria 3-7). With the aid of the 1980 Canadian emissions inventory compiled by the Environmental Protection Service in Canada[5] the proximity to and strength of emission sources were determined. With only minor violations to the criteria in Table 4, five of the twenty-nine CANSAP sites and five of the seven APN sites fell into the representative category. Thus the stringent criteria in Tables 4 label most of the Canadian sites potentially unrepresentative and leave too few sites for evaluation purposes. When the

available, is shown by a number. A few sites have co-located samplers. For these sites two levels of observations are given, one for each sampler. The associated wet deposition amounts are not given, since in the ISDME project observed data will not be made available to modellers prior to computing deposition amounts.

Conclusions and Recommendations

The evaluation of LRT sulfur models requires high quality wet deposition data with estimates of uncertainties. Unfortunately, the uncertainties have yet to be quantified. As an alternative, the regional representativeness of precipitation chemistry sites and the reliability of network data have been classified into three levels of uncertainty. In addition, a method of screening the precipitation chemistry data and determining the wet deposition amount from five North American precipitation chemistry networks has been recommended.

Based on the adopted screening criteria less than thrity percent of the observations fell into level 1, i.e. the level of least uncertainty. The most frequent reasons for failing this level were potentially unrepresentative siting, poor collection efficiency and poor data capture.

The approach for estimating wet deposition amounts in the ISDME is refined and extended by the "Unified Data Base Committee" established under RMCC/ASSG. It is recommended that other users will follow this committee's approach for estimating wet deposition. It is also recommended that the uncertainties in the measurements be quantified. To reduce uncertainties, it is recommended that the ongoing review of the siting and operations of the monitors be continued. In Canada the siting problem has been reviewed and resulted in the CAPMoN network.

Acknowledgement

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TABLE 1: DATA SCREENING CRITERIA FOR ANNUAL CONCENTRATION/DEPOSITION

	Criterion	Level 1	Level 2	Level 3
(1)	Siting	Regionally Representative	Representative	Representative or Unrepresentative
(2)	Seasalt Correction (for sulfate)	$\leq$ 25%	$\leq$ 50%	$\leq$ 75%
(3)	Overall Collector Efficiency	$\geq$ 60% (75)^{o}	$\geq$ 50% (> 50)^{o}	$\geq$ 40% (> 40)^{o}
(4)	No. of Samples			
	- monthly/28-day	$\geq$ 10+	$\geq$ 10+	$\geq$ 8+
	- weekly	$\geq$ 40+	$\geq$ 40+	$\geq$ 34+
	- daily/event	$\geq$ 80%*	$\geq$ 80%*	$\geq$ 60%*
(5)	No. of Samples During Each Season			
	- monthly/28-day	$\geq$ 2+	$\geq$ 2+	$\geq$ 1+
	- weekly	$\geq$ 10+	$\geq$ 10+	$\geq$ 4+
	- daily/event	$\geq$ 60%*	$\geq$ 60%*	$\geq$ 40%*

TABLE 2: DATA SCREENING CRITERIA FOR WINTER SEASON

	Criterion	Level 1	Level 2	Level 3
(1)	Siting	Regionally Representative	Representative	Representative or Unrepresentative
(2)	Seasalt Correction (for sulfate)	$\leq$ 25%	$\leq$ 50%	$\leq$ 75%
(3)	Overall Collector Efficiency	$\geq$ 40% (>75)^{o}	$\geq$ 20% (> 50)^{o}	$\geq$ 20% (> 40)^{o}
(4)	No. of Samples			
	- monthly/28-day	$\geq$ 2+	$\geq$ 2+	$\geq$ 1+
	- weekly	$\geq$ 10+	$\geq$ 10+	$\geq$ 4+
	- daily/event	$\geq$ 60%*	$\geq$ 60%*	$\geq$ 40%*

\+ Dry collection periods are also included in this number
o The bracketed value applied to U.S. data
* Based on total number of events, as determined from co-located standard gauge

TABLE 3: DATA SCREENING CRITERIA FOR SPRING, SUMMER AND FALL

	Criterion	Level 1	Level 2	Level 3
(1)	Siting	Regionally Representative	Representative	Representative or Unrepresentative
(2)	Seasalt Correction (for sulfate)	$\leq$ 25%	$\leq$ 50%	$\leq$ 75%
(3)	Overall Collector Efficiency	$\geq$ 75%	$\geq$ 50%	$\geq$ 40%
(4)	No. of Samples			
	- monthly/28-day	$\geq$ 2+	$\geq$ 2+	$\geq$ 1+
	- weekly	$\geq$ 10+	$\geq$ 10+	$\geq$ 4+
	- daily/event	$\geq$ 60%	$\geq$ 60%*	$\geq$ 40%*

\+ Dry collection periods are also included in this number
* Based on total number of events, as determined from co-located standard gauge

TABLE 4: SITING CRITERIA FOR REGIONALLY REPRESENTATIVE MONITORS

1. There is no continuous industrial source, town or suburban area located within 10 kilometres.

2. There is no major point source (> 10,000 tons sulfur dioxide per year) located within 50 kilometres; or the sum of point source emissions within 50 kilometres is less than 10,000 tons per year.

3. There is no surface pollutant storage facility (e.g. salt pile) located within 1 kilometre.

4. There are no major transportation sources, furnaces or incinerators located within 100 metres.

5. There is no cultivation or other intensive agricultural acitivity within 500 metres.

6. There is no building, tree, etc. to impinge on the cone defined by a 30° angle above the horizontal plane and centred at the site.

7. The local area is not dusty, i.e. the ground cover is good.

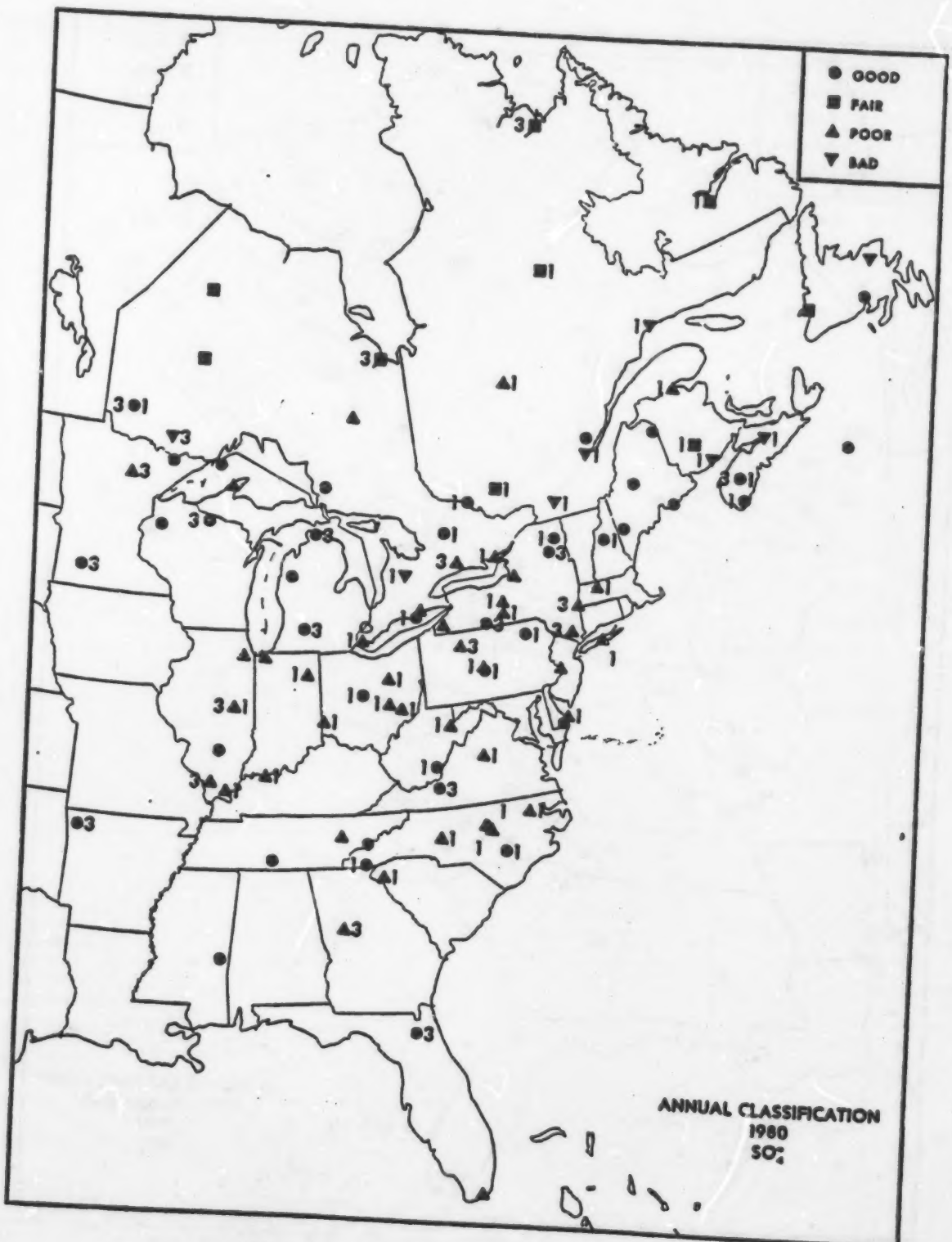

Figure 1. Rating of sites and levels of observations for 1980.

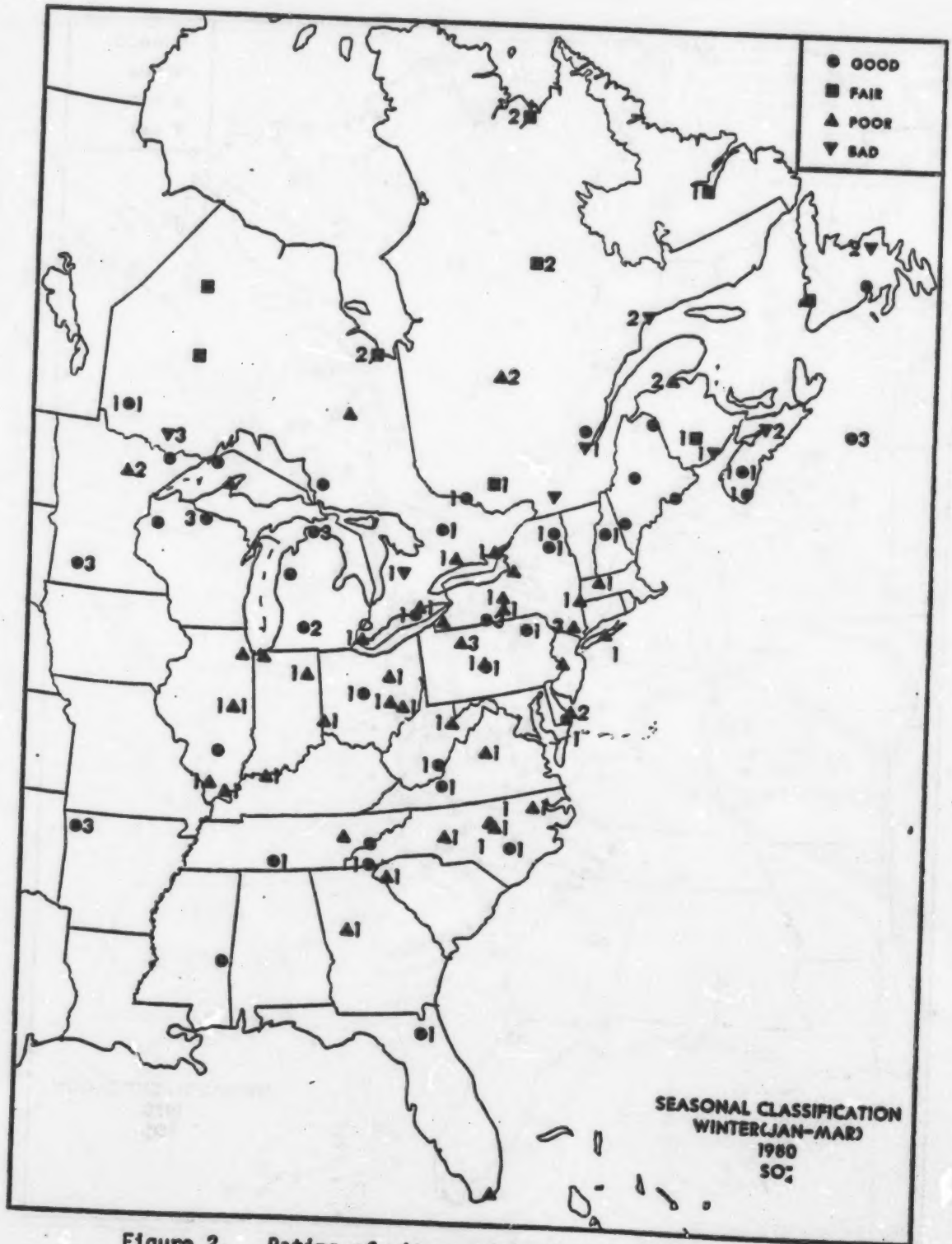

Figure 2. Rating of sites and levels of observations for winter.

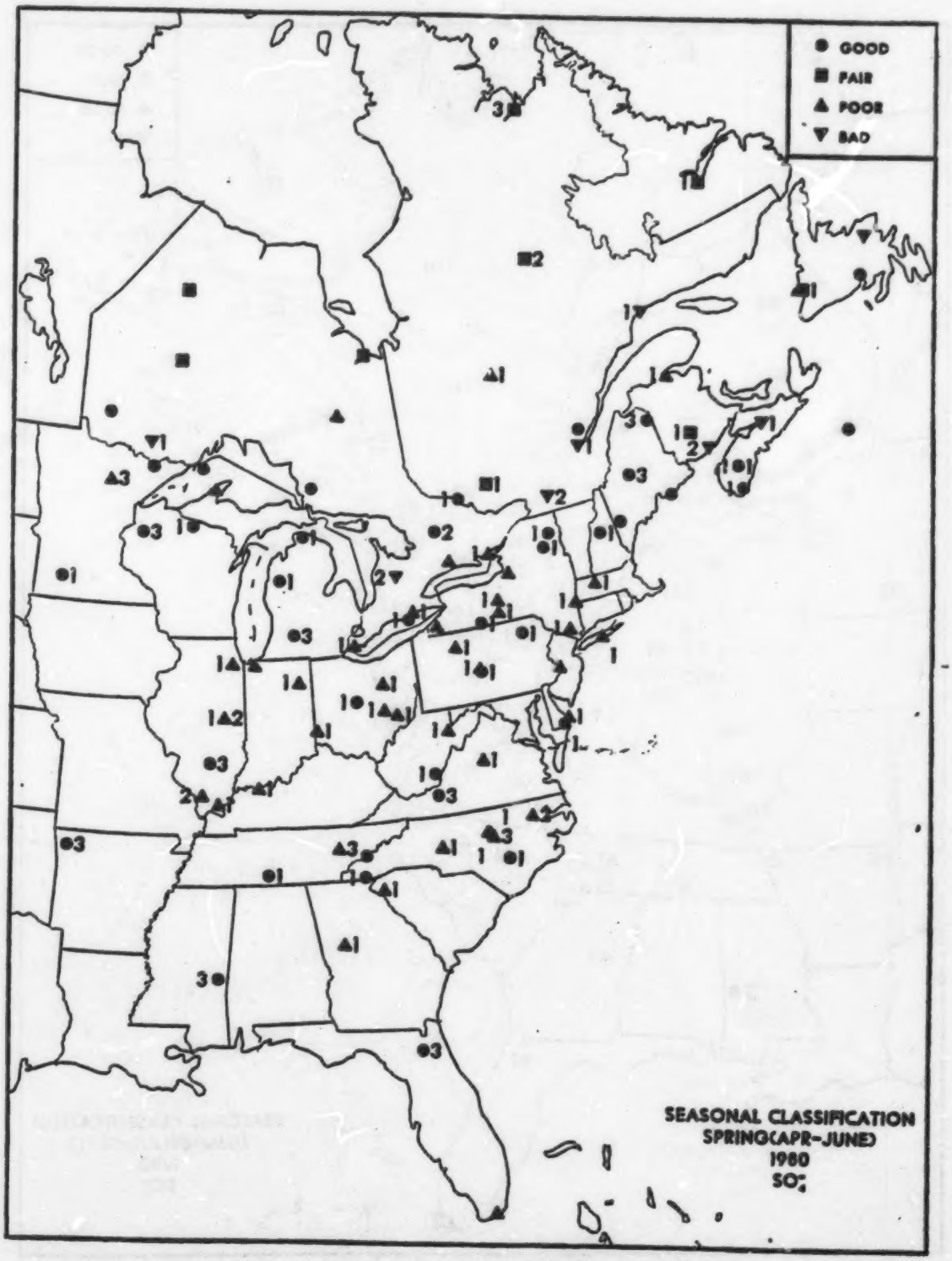

Figure 3. Rating of sites and levels of observations for spring.

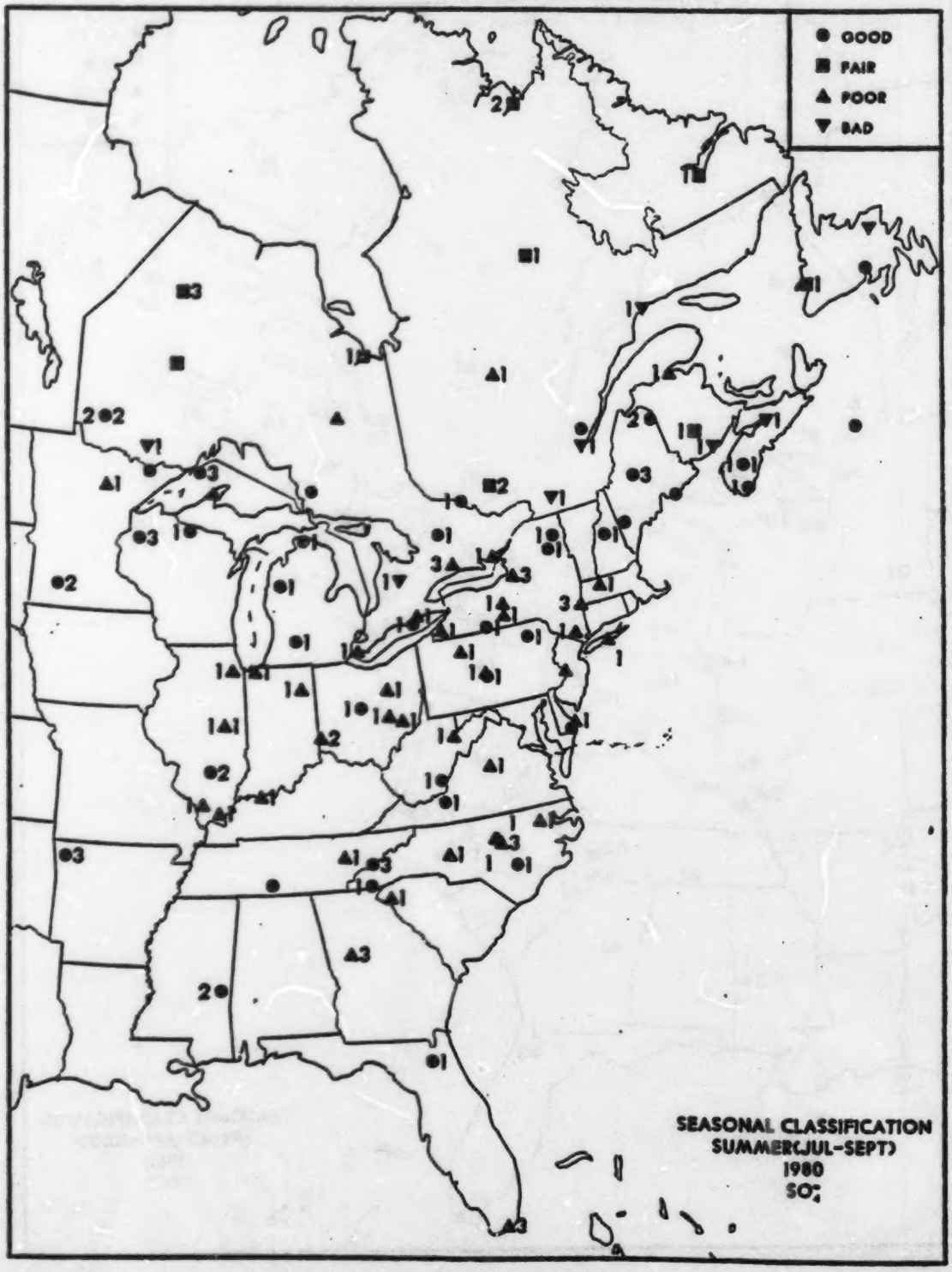

Figure 4. Rating of sites and levels of observations for summer.

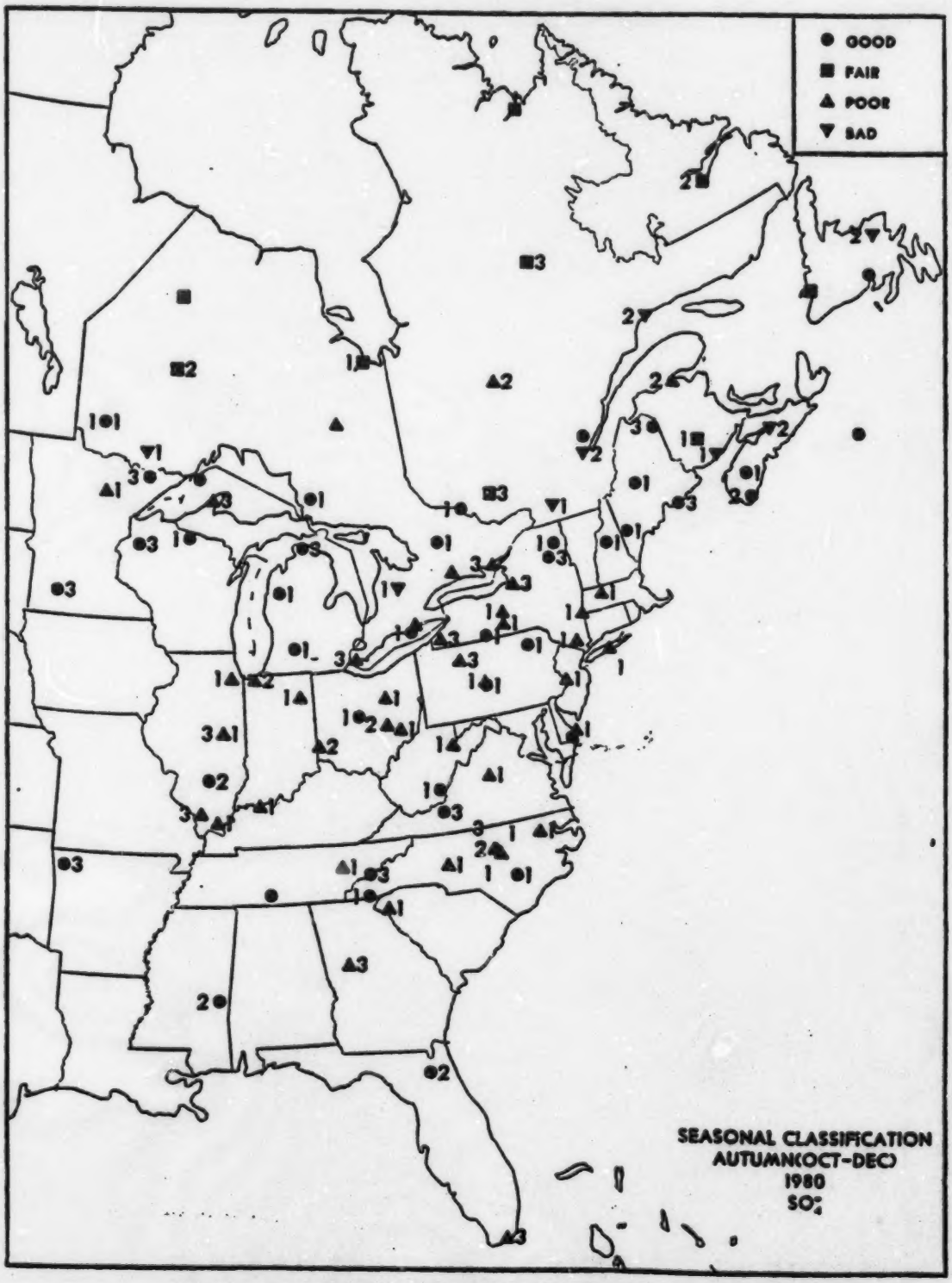

Figure 5. Rating of sites and levels of observations for fall.